Solid-State NMR BMRB Deposition Content – Draft Specification (04/10/2005)

The outline below is a draft description of information unique primarily to a solid-state NMR study of a biomolecular system that could be included in a BMRB deposition. The chemical structure of the system studied, a citation for the deposition, and other general information would also be included in a full deposition. Atomic coordinates and restraints for a structure determination could be part of a deposition in the future and would be forwarded to the PDB. This draft is the result of the work of Dr. Matsuki and Professor Akutsu from Osaka University in collaboration with the BMRB staff.

Input on these specifications from the solid-state NMR community is essential to developing a complete and efficient archive of solid-state NMR data at BMRB. An electronic version of this document will be available from the BMRB web site at this URL:

http://www.bmrb.wisc.edu/bmrb/features/

Please take the time to review this draft and send your comments and suggestions to Eldon Ulrich at BMRB (elu@bmrb.wisc.edu). Suggestions on the specific content of the archive and on which data items should be required for a complete solid-state NMR entry are critical.

1. Kinds of experimental data or derived results archived

1.1. NMR parameters

- 1.1.1. Assigned chemical shifts
- 1.1.2. Chemical shift referencing
  - 1.1.2.1. Primary reference compound
  - 1.1.2.2. Shift for secondary reference compound (hexamethyl benzene, adamantane, etc.)
  - 1.1.2.3. Concentration and solvent for primary reference (DSS in water, TMS in chloroform, neat TMS, etc.)
  - 1.1.2.4. Δδ between primary and secondary reference used to report chemical shifts
- 1.1.3. Dipolar coupling results
  - 1.1.3.1 Scaling factor of the recoupling sequence
  - 1.1.3.2. Fitting procedure
- 1.1.4. Quadrupolar coupling
- 1.1.5. Tensors
  - 1.1.5.1. Chemical shift
    CSA, asymmetry, principal components, Euler angles
  - 1.1.5.2. Quadrupolar
  - 1.1.5.3. Dipolar

1.2. Molecular geometries

- 1.2.1. Bond orientations with respect to Bo
- 1.2.2. Molecular axis with respect to Bo
- 1.2.3. Secondary structural elements (from chem. shifts)

2. Supporting data archived

2.1. Sample description

- 2.1.1. Type (lyophilized powder, polycrystalline powder, single crystal, fibrous protein, oriented glass plate/membrane film, precipitated microcrystal)
- 2.1.2. Content (weight and other characteristics of sample components)
  - 2.1.2.1. Biopolymers (isotopic labeling pattern – single site, methyl group, other side chain specific labeling, uniform, SAIL)
  - 2.1.2.2. Excipients (salts, stabilizing agents, etc.)
- 2.1.3. Preparation
  - 2.1.3.1. Crystallization (procedure followed, solution contents, etc.)
  - 2.1.3.2. Cryo-protectant, if used
  - 2.1.3.3. Oriented sample (procedure followed)

2.2. Sample conditions

- 2.2.1. Temperature
  - 2.2.1.1. Controller setting
  - 2.2.1.2. Actual internal temperature
  - 2.2.1.3. Calibration agent

2.3. Experimental parameters

- 2.3.1. Spectrometer parameters
  - 2.3.1.1. Field strength
  - 2.3.1.2. Rotor frequency
  - 2.3.1.3. Rotor angle
  - 2.3.1.4. Spectrometer manufacturer
  - 2.3.1.5. Spectrometer model
- 2.3.2. Pulse programs (This information could be deposited for each NMR experiment that was carried out.)
  - 2.3.2.1. Overall experiment
  - 2.3.2.2. Recoupling sequence
    - 2.3.2.2.1. Name (RFDR, SPC5, etc.)
    - 2.3.2.2.2. Type (homonuclear or heteronuclear)
    - 2.3.2.2.3. Nuclei
    - 2.3.2.2.4. Time period for first mixing time
  - 2.3.2.3. Decoupling sequence
    - 2.3.2.3.1. Name
    - 2.3.2.3.2. Nuclei
    - 2.3.2.3.3. Time period
    - 2.3.2.3.4. Decoupling strength (kHz)
  - 2.3.2.4. Citation for the pulse program
- 2.3.3. Probe parameters
  - 2.3.3.1. Rotor characteristics
    - 2.3.3.1.1. Diameter
    - 2.3.3.1.2. Length
    - 2.3.3.1.3. Volume (uL)
    - 2.3.3.1.4. Composition (zirconium, etc.)
    - 2.3.3.1.5. Spacer (yes/no)?
- 2.3.4. Probe characteristics
  - 2.3.4.1. Type (transmission line, home built, triple/double resonance, inverse coil, solenoid/saddle, etc.)